Coupled THM Simulations of the Drift Scale Test at Yucca Mountain

S.C. Blair, S.R. Carlson, and K. Lee

March 8, 2002

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

This report has been reproduced directly from the best available copy.

Available electronically at http://www.doc.gov/bridge

Available for a processing fee to U.S. Department of Energy
And its contractors in paper from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-mail: reports@adonis.osti.gov

Available for the sale to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-mail: orders@ntis.fedworld.gov
Online ordering: http://www.ntis.gov/ordering.htm

OR

Lawrence Livermore National Laboratory
Technical Information Department's Digital Library
http://www.llnl.gov/tid/Library.html

Coupled THM Simulations of the Drift Scale Test at Yucca Mountain

Stephen C. Blair
Geophysics and Global Security Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

Steven R. Carlson
Geophysics and Global Security Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

Kenrick Lee
Geological and EnvironmentalTechnology Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

Jeffery L. Wagoner
Geological and EnvironmentalTechnology Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

ABSTRACT: This paper presents a coupled thermal-hydrological-mechanical (THM) analysis of the Drift Scale Test (DST) conducted at Yucca Mountain, Nevada. The DST is a large-scale, long-term thermal test designed to investigate coupled thermal-mechanical-hydrological-chemical behavior in a fractured, welded tuff rock mass in support of nuclear waste isolation efforts. The model used for this analysis utilizes temperature distributions predicted by a thermal-hydrological code as input to a distinct element thermal mechanical code. This paper presents a brief discussion of the test and the coupled model, followed by comparison of predicted and measured displacements. Results show that the model predicts the trend and magnitude of the displacements observed in a cross section monitored in the test through four years of heating. Maximum principal stress levels of 60 MPa are predicted in the crown and floor of the heated drift (HD) after 4 years of heating. Comparison of predicted and observed displacements shows that the model closely predicts vertical displacement above the HD and provides a good estimate of horizontal displacement perpendicular to the HD. These results indicate that a thermal expansion coefficient of 9e-6/°C is generally appropriate for the rockmass forming this test. Normal displacements on joints in the cross section examined here show opening of up to 2mm on subvertical fractures in regions above and below the HD after 4 years of heating. These fractures do not close upon cooldown, indicating that some permanent enhancement of vertical fracture permeability may occur.

1. INTRODUCTION

The Yucca Mountain Site Characterization Project is conducting a drift scale heater test, known as the Drift Scale Test (DST) at Yucca Mountain, Nevada. The DST is a large-scale thermal test designed to investigate coupled behavior in a fractured, welded tuff rock mass over a period of eight years [1].

We have used a coupled thermal-hydrological-mechanical (THM) model to analyze the geomechanical response of the rock mass forming the DST. This model utilizes temperature distributions predicted by the NUFT thermal-hydrological code [2] as input to the 3DEC distinct element thermal mechanical code [3]. This work is an extension of the work presented by Blair, et al at DC Rocks [4]. Results presented here include comparison of measured and predicted displacements, estimates of joint normal displacement and estimates of the stress field around the heated drift (HD).

It is important to note that the model used here has been developed for analysis of thermal-mechanical (TM) effects on hydrological properties of a fractured rock mass around emplacement drifts, and in the pillar between drifts in a potential geologic repository for radioactive waste. The analysis of the DST presented here represents part of the validation and confidence building efforts for the coupled model.

2. DESCRIPTION OF THE DST

The DST is being conducted in an alcove of the Exploratory Studies Facility (ESF) at Yucca Mountain, Nevada. This test is sited in a fractured, densely welded ash-flow tuff that forms part of the Topopah Spring Tuff member of the Paintbrush Group. Fractures form the primary conduits for fluid flow in the rock mass. The general layout of the DST is shown in Figure 1. The heated drift (HD) is 5m in diameter and approximately 60 m long. Access to the HD from the ESF is gained through the Access Observation Drift (AOD) and a

heaters located in the HD, and wing heaters in 50 boreholes perpendicular to the HD. These wing heater holes are spaced at 2-m intervals along each rib of the HD. The wing heaters extend into the rock approximately 11 m from the rib. Together, these heaters provided approximately 180 kW of power to heat a region of rock that is roughly planar and approximately 50 m long and 27 m wide. The test involves 4 years of heating followed by a 4-year cool-down period [1]. The heating portion of the DST was started in December 1997, and the target temperature of 200ºC was reached in the crown of the HD in summer 2000. The heater power was adjusted periodically so as to maintain 200ºC in the crown for the duration of the heating phase. Deformation of the rock mass is being monitored with an array of multiple-point borehole extensometer (MPBX) systems. Locations of the MPBX boreholes are shown in Figure 1. These boreholes represent only a small fraction of the boreholes drilled into the DST for emplacement of various types of instrumentation that enable temperature, geophysical, hydrological, and chemical measurements [1].
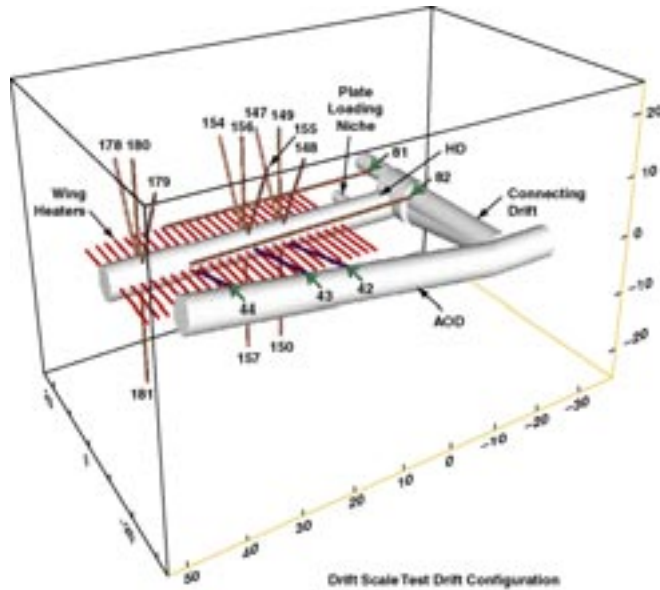

Figure 1. DST layout showing drifts, wing heaters and boreholes for mechanical measurements.

3. MODEL FORMULATION

We have formulated a coupled THM model for simulation of THM processes in fractured rock masses. This model uses the NUFT finite difference code for thermal hydrologic analysis, and the 3DEC distinct element code for thermal mechanical analysis. The model is described in detail in

the lifetime of the test. The temperatures are input to 3DEC, which then computes stresses and deformations at the selected times. The distinct element method permits the inclusion of discrete fractures, so that fracture deformation and associated stress redistribution can be accommodated.

The model setup for the DST simulations incorporates the detailed geometry of the excavations forming the DST as shown in Figure 2. Fractures included in the model are listed in Table 1 and are shown in Figure 3. This fracture set was derived from a data set of fractures mapped in the DST block [4,5].
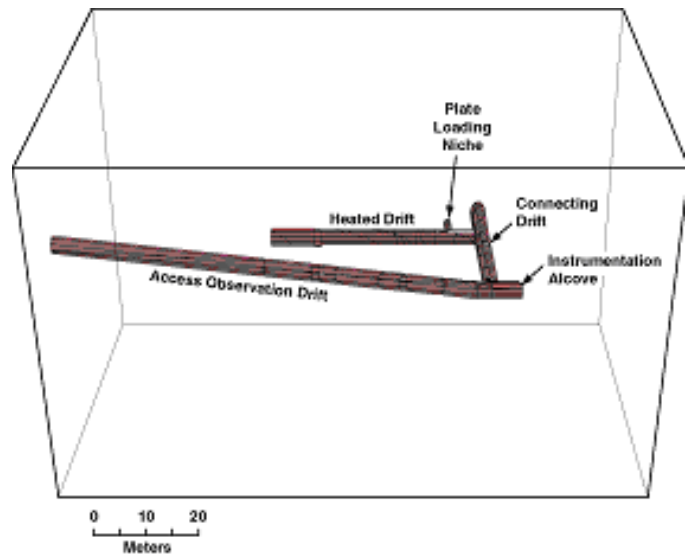

Figure 2. Model domain showing excavations.

Table 1. Coordinates of fractures used in analysis.

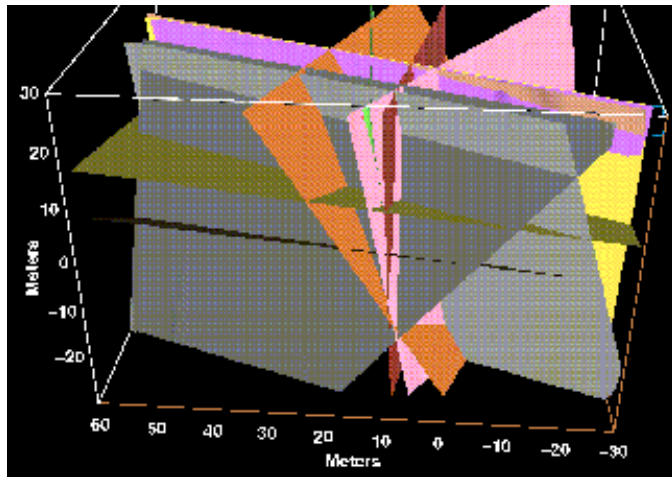| Frac No	Dip Dir (°)	Dip (°)	X coord (m)	Y coord (m)	Z coord (m)
1	199	75	−21.40	−8.26	4.11
2	86	83	−12.86	−10.11	−3.93
3	122	61	−13.52	−9.70	−1.38
4	28	13	−4.91	−8.32	5.57
5	51	6	−1.87	−6.60	6.35
6	9	31	−25.79	−8.20	1.57
7	21	62	−9.70	−6.54	5.51
8	20	84	−3.32	−8.33	5.71
9	22	68	−1.57	−8.28	16.26
10	20	82	−3.59	−6.59	6.17
11	20	84	−15.50	−8.28	4.63
12	124	81	−22.44	−8.17	0.58
13	100	88	−16.81	−8.13	−1.08

Figure 3. Model domain showing fracture distribution.

Temperatures were input at a series of 30 times during the period from 0 - 15 years (5475 days) from the start of heating. The times were selected to capture the initial thermal response of the rock to heating as well as the longer-term steady evolution of the temperature field.

Boundary conditions were applied to the simulated rock mass as follows. The base of the model was considered to be a roller boundary so that only horizontal displacements were allowed. The top of the rock mass, and vertical sides parallel to the HD were modeled as stress boundaries, while the vertical sides perpendicular to the HD were modeled as roller boundaries, allowing no horizontal displacement perpendicular to the face. An in situ stress condition was applied with a vertical stress of 5.54 MPa and a horizontal stress of 4.85 MPa on the vertical sides parallel to the HD. Stress gradients were 0.021 MPa per meter of depth for vertical stresses and 0.0115 MPa per meter of depth for horizontal stresses. A simulation was also conducted with all four vertical sides configured as stress boundaries. Comparison of simulated and measured displacements showed that the latter boundary condition underestimated the displacement in direction parallel to the drift.

Rock properties for the simulation are summarized in Table 2. These values are identical to those used for emplacement drift simulations in the TSw2 unit at Yucca Mountain [5].

4. RESULTS

This section presents results of displacement observations and of simulations of the THM behavior during heating, and predictions of THM

Prior to the excavation of the Heated Drift (HD) three boreholes were drilled from the Access and Observation Drift (AOD) perpendicular to the planned location of the Heated Drift. These boreholes (numbered 42, 43, and 44 in Figure 1) were instrumented with MPBX systems and deformations were recorded during the excavation of the Heated Drift. The borehole responses due to the drift excavation were simulated using the model, and can be used to evaluate the bulk and shear moduli of the rock mass in the simulation.

Table 2. Rock properties used for DST simulation.

Description	Value	Units
Matrix Properties		
Dry Bulk Density	2270	kg/m³
Intact Rock Elasticity Modulus	33.03	GPa
Coefficient of Thermal Expansion	9.73E-6	1/°C
Rock Mass Elasticity Modulus	24.71	GPa
Rock Mass Bulk Modulus	14.2	GPa
Rock Mass Shear Modulus	10.2	GPa
Poisson's Ratio	0.21	None
Joint Properties		
Joint Tensile Strength	0	MPa
Joint Friction	41	Deg
Joint Cohesion	0.09	MPa
Joint Normal Stiffness	98.1	MPa/mm
Joint Shear Stiffness	40.5	MPa/mm
Joint Dilation Angle	29	Deg
Boundary and In Situ Stresses		
In Situ Stress (280 m depth)	5.54	MPa
Vertical Stress Gradient	0.021	MPa/m

The excavation of the HD was simulated by excavating the entire length of the HD at one time. Thus the time history of the HD excavation was not simulated, but the effect of the excavation on the rock surrounding these boreholes was determined.

The deformations of the deepest anchors in holes 42 and 43 were simulated and the resulting total deformations are listed in Table 3 along with total deformations measured by the MPBX systems. These data are plotted in Figure 4. This table shows good agreement between the observed and predicted displacements (within a factor of 2). Borehole 44 was not used in this analysis as the data for this borehole were judged to be of poor quality.

Table 3. Deformation Due to Mine-by of HD

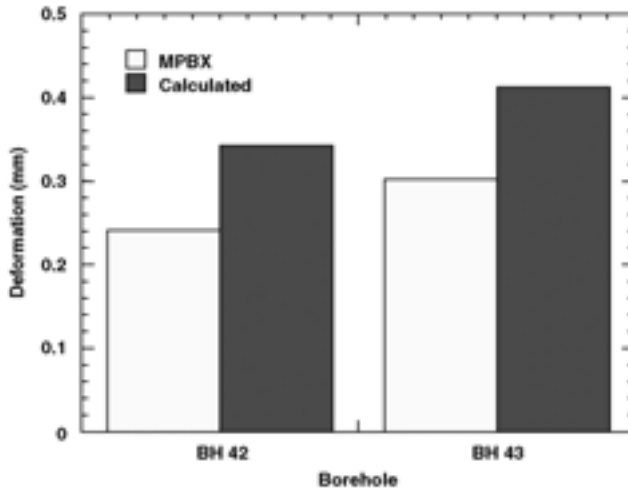| Borehole	Anchor 6 Observed (mm)	Anchor 6 Predicted (mm)
42	2.4	3.5
43	3.1	4.1

Figure 4. Total deformation for boreholes 42 and 43 during mine-by, prior to heating

4.2 Comparison of Observed and Predicted Displacement During Heating

MPBX instrumentation in boreholes 147, 148 and 149 monitor displacement in the roof of the HD along a cross section 13 m from the bulkhead (see Figure 1). Anchors were placed at depths of 1, 2, 4, and 15 m in these boreholes. Anchors at 4 and 15 m are denoted as anchors 3 and 4, respectively. Simulated displacements for anchors 3 and 4 in these holes are shown along with observed displacements in Figure 5 a-c. These displacements are referenced to the borehole collar in the roof of the drift. Noise in the MPBX data is due to boiling /refluxing of water in the boreholes, which were not sealed. These figures show that (as expected) most of the displacement occurs in the first 4 m of the borehole, where the rock is the hottest. Also, at early times (<500 days) anchor 3 displaces more than anchor 4, indicating compression of the rock between anchor 3 and 4 during this period. This behavior is also shown in the model. The predicted response of anchor 3 in these holes closely matches the observed behavior. The predicted response of anchor 4 lags the observed response at times less than 200 days. The observed response of anchor 4 in these holes is correlated with temperature near

the anchor location. This lag in behavior of the anchors at distance from the heaters was also observed in the deformation data for the Large Block Test [6], also conducted in support of nuclear waste storage at Yucca Mountain. Note that the data showing a drop in displacement for BH 147 just after 1000 days (Figure 5a) are considered unreliable and are included here for completeness.
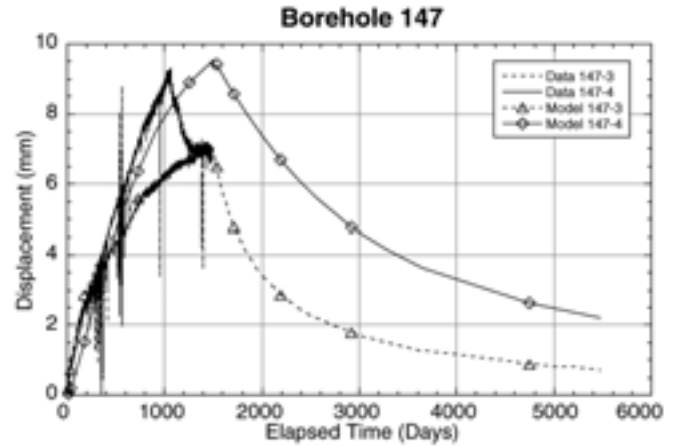

Figure 5a. Observed and predicted displacement for anchors 3 and 4 in borehole 147 (angled 30° away from the AOD).
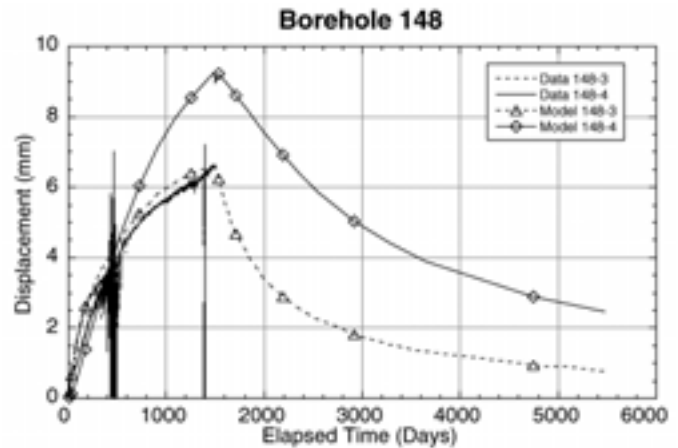

Figure 5b. Observed and predicted displacement for anchors 3 and 4 in borehole 148 (angled 30° toward the AOD).
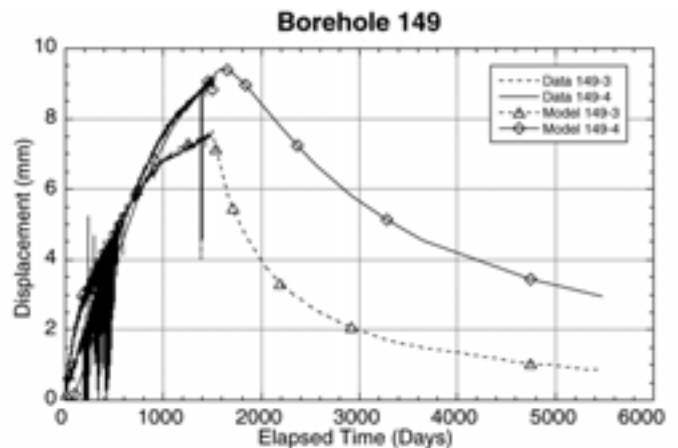

Figure 5c. Observed and predicted displacement for anchors 3 and 4 in borehole 149 (vertically up).
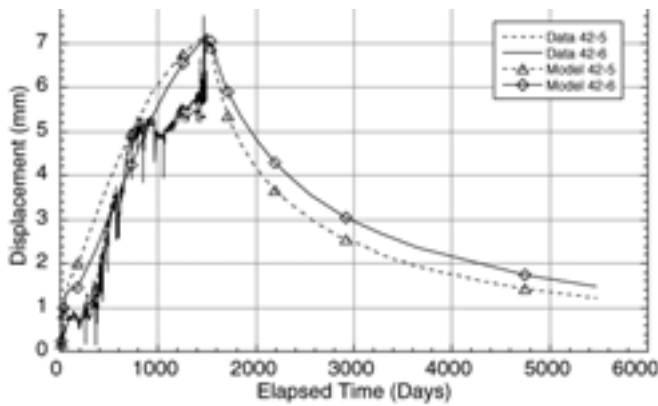
Figure 6. Observed and predicted displacements for borehole 42 (subhorizontal).

Borehole 42 monitors deformation in the horizontal direction between the AOD and the HD at 13 m from the bulkhead. Observed and predicted displacements for anchors 5 and 6 at 11.6 and 13.6 m from the HD in this borehole are shown in Figure 6. Note that these deformations are referenced to an anchor at the bottom of the borehole nearest the HD. The field data show nearly identical displacement for the two anchors, indicating that the anchors moved as a rigid body, with very little thermal expansion. While the model captures the general trend and magnitude of the deformation, it overpredicts the initial response.

These figures show that the model captures the overall trend and magnitude of the observed displacement in the cross section at 13 m from the bulkhead. Comparison of measured and predicted displacements for other cross sections show similar agreement. This result indicates that the value of coefficient of thermal expansion (CTE) of 9.73E-6/°C is appropriate for the DST rockmass. This value was determined from laboratory measurements on intact samples [7]. This is significantly higher than the value of 5.27 E-6/°C measured in the Single Heater Test, which was also conducted in Alcove 5 [8]. Moreover, Lin et. al [6] found that the lower value provided a good fit to displacement observations in the LBT, and that the higher value used here overpredicted the observed displacement. The reason for this discrepancy is not known at the present time.

The model also captures the slight anisotropy in the displacement, as both the data and the model indicate slightly larger displacements on the non-AOD side of the HD (Figure 5a) than on the AOD side (Figure 5b).

The overall displacement field after approximately 4 yr (1503 days) of heating, for a cross section at 13 m from the bulkhead, is shown in Figure 7. Also shown on this figure are locations of the heated drift wing heaters and the AOD, as well as boreholes 147 – 149 in the roof of the HD. This figure shows that the largest displacements are vertical and subvertical and occur above the heaters in a region starting about 2 drift diameters above the heater plane. The plot also shows the slight anisotropy in the deformation with slightly larger displacements on the side of the HD away from the AOD, and smaller displacement to the outside of the AOD. Note that the deformations plotted in this figure are referenced to initial locations in the model, prior to drift excavation and heating, thus the individual values are not in exact agreement with the observed values.

The predicted joint normal displacements after 4 yr of heating in the cross section at 13 m from the bulkhead are shown in Figure 8. This figure indicates that at this cross section fracture dilation of up to 2 mm is predicted for vertical and subvertical fractures in areas more than 2 drift diameters above and below the HD.

Note that the model shows very little joint normal displacement in the region between the HD and the AOD (see Figure 8). A series of pneumatic permeability measurements made in this region [1], show very little change in fracture permeability. This is consistent with the prediction of minimal fracture deformation in this region. Moreover, this result shows that DEM analysis may be useful in the design of future measurement and/or monitoring systems.

The good agreement between the observed and predicted displacements indicates that the stress field predicted by the model may provide a reasonable approximation to the actual stress field in the rock. This is useful because stress measurement was not incorporated into the DST design. Analysis of the stress field predicted by the model indicates that the maximum principal stress near the drift rotates from vertical to horizontal during the heating phase of the test. Figure 9 presents contours of the horizontal stress component in the direction perpendicular to the drift at 1503 days. This figure indicates that horizontal stress levels above 60 MPa may have occurred in the rock within 1 drift diameter of the HD. Moreover, as discussed above, rock in this region was held at or near 200 °C for approximately 1.5 years. Under
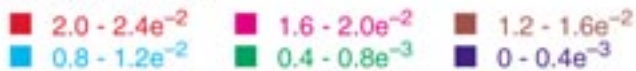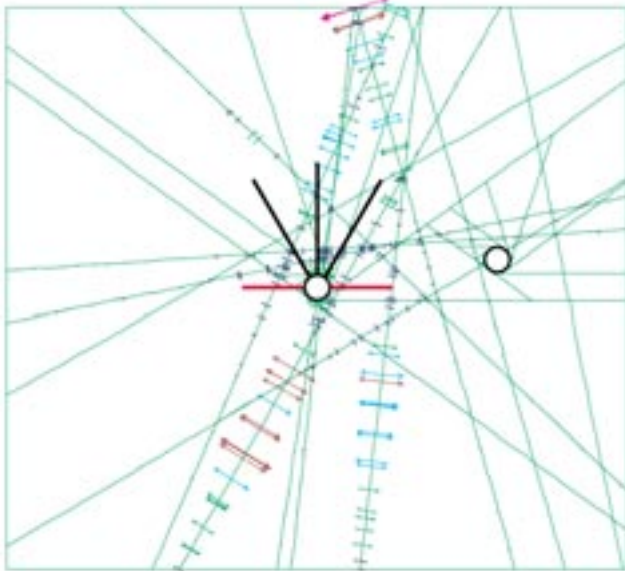
Displacement (m)

- 2.0 - 2.4e^{-2}
- 1.6 - 2.0e^{-2}
- 1.2 - 1.6e^{-2}
- 0.8 - 1.2e^{-2}
- 0.4 - 0.8e^{-3}
- 0 - 0.4e^{-3}
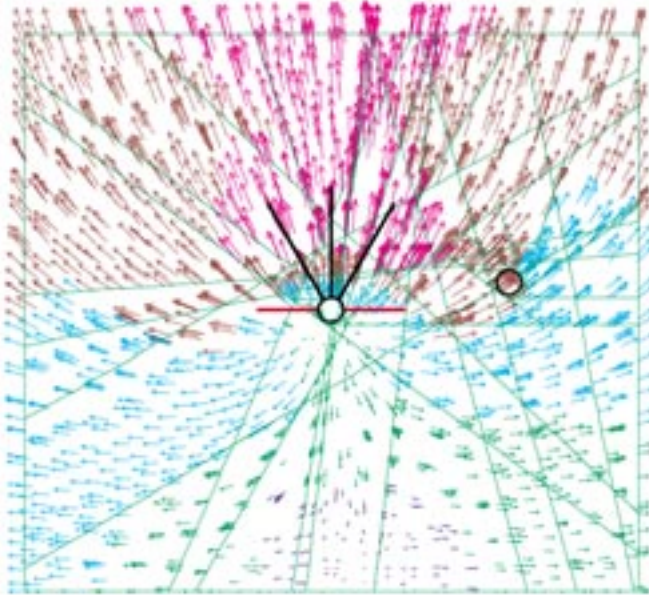
Figure 7. Displacement vectors in plane 13 m from bulkhead after 4 years of heating.

Stress (Pa)

- 5 - 6e^7
- 4 - 5e^7
- 3 - 4e^7
- 2 - 3e^7
- 1 - 2e^7
- 0 - 1e^7

Figure 9. Horizontal stress distribution for cross section 13 m from bulkhead after 4 years of heating.

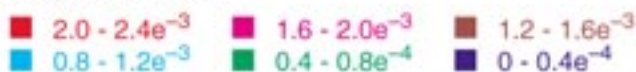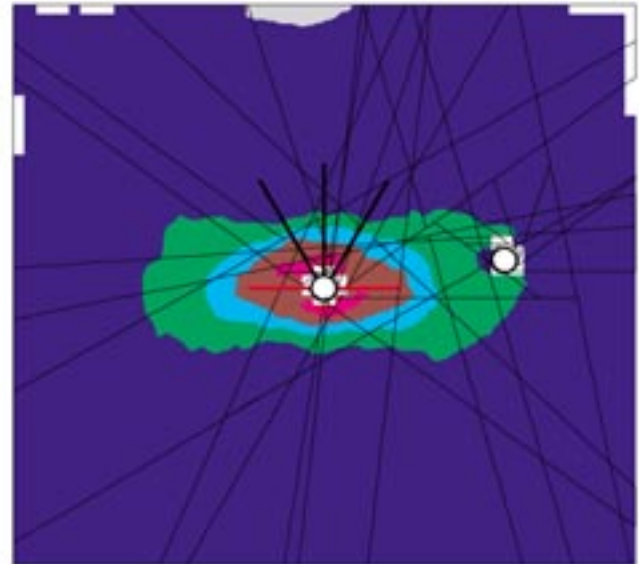Joint Normal Displ. 1503 Days
- 13 m West of Bulkhead

Displacement (m)

- 2.0 - 2.4e^{-3}
- 1.6 - 2.0e^{-3}
- 1.2 - 1.6e^{-3}
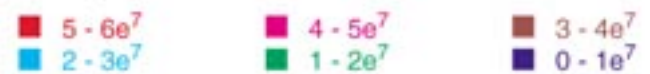- 0.8 - 1.2e^{-3}
- 0.4 - 0.8e^{-4}
- 0 - 0.4e^{-4}

Figure 8. Joint normal displacement for cross section 13 m from bulkhead after 4 years of heating.

Figure 10. Heated Drift Crown at about 3 m in from bulkhead after 3.5 years of heating.

these conditions, spalling of the rock can be expected as 60 MPa is approximately one half of the uniaxial compressive strength of the intact rock. Figure 10 shows that slabbing of the roof has occurred. This figure shows dinner plate sized rock slabs that have spalled off the roof and are held by wire mesh. This was noticed in June 2001, and to date no further slabbing has been observed.
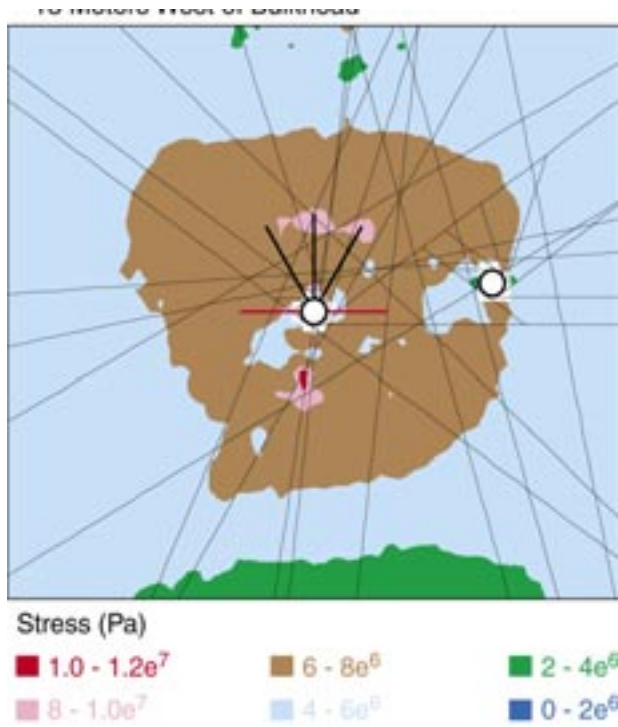
Stress (Pa)

■ 1.0 - 1.2e^7	■ 6 - 8e^6	■ 2 - 4e^6
■ 8 - 1.0e^7	■ 4 - 6e^6	■ 0 - 2e^6

Figure 11. Horizontal stress distribution for cross section 13 m from bulkhead after 11 years of cooling.

Displacement (m)

■ 2.0 - 2.4e^{-3}	■ 1.6 - 2.0e^{-3}	■ 1.2 - 1.6e^{-3}
■ 8.0e^{-4} - 1.2e^{-3}	■ 4 - 8e^{-4}	■ 0 - 4e^{-4}

Figure 12. Joint normal displacement for cross section 13 m from bulkhead after 11 years of cooling.

4.4 Cooldown Predictions

The predicted behavior of rock above the HD during cooldown is shown for boreholes 147 – 149 in Figures 5 a–c. These figures show that contraction during cooling is predicted to be greatest within the first 4 m of rock as shown by the behavior of anchor 3 in these plots. Moreover, anchor 3 is predicted to recover most of the displacement in the first 4 years of cooling (1500 –3000 days). These figures also show that recovery for rock 15 m from the drift wall (anchor 4) is slower and not as complete, indicating some hysteresis may occur in the thermally induced displacement between 4 and 15 m into the drift roof. The horizontal stress field predicted for this cross section after 11 years of cooling is shown in Figure 11. This figure shows that at this time stress levels have returned to near ambient. Figure 12 presents predicted joint normal displacements after 11 years of cooling for the cross section at 13 m from the bulkhead. This figure is nearly identical to Figure 6 and indicates that vertical fractures that open during heating are not predicted to recover during cooldown. This implies that enhanced fracture permeability, formed during heating, may persist through the cooldown phase. Thus, the simulations indicate that significant displacement will remain in the rock even after the stress field has dissipated due to cooling.
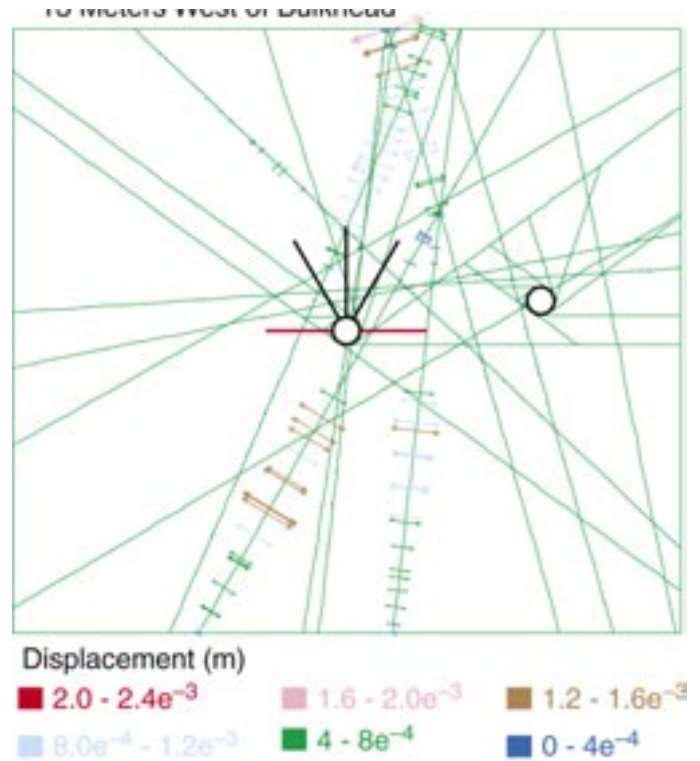
5. CONCLUSIONS

A distinct element analysis has been developed to estimate the thermal mechanical effects on fracture permeability in the rock mass for the Drift Scale Test. The following conclusions have resulted from this analysis: First, comparison of predicted and measured displacements in cross sections of the DST indicates that the model predicts the trends and magnitudes of the measurements very well through the end of the heating phase. Results indicate that a CTE of 9.73 E-6/°C is appropriate for the DST. After 4 years of heating, the highest displacements are predicted for a zone directly above the HD and wing heaters, and a few drift diameters above the heater plane. Predicted joint deformations indicate that vertical and subvertical joints will open in zones located above and below the HD, and a few drift diameters into the rock mass. Fractures form the primary conduits for fluid flow in the rock mass and fracture permeability is strongly dependent on fracture deformation. The results for joint normal displacement indicate that drainage through fractures may be enhanced in regions a few drift diameters above and below the HD.

During the heating phase, the thermal mechanical processes are predicted to have rotated the principal stress direction from primarily vertical to primarily horizontal, oriented perpendicular to the heated drift

the drift. This combination of stress and temperature has caused spalling in the roof of the HD.

Predictions for cooldown behavior indicate that the stress field will return to near ambient within 11 years of the end of heating, but that significant displacement may remain. In particular, normal opening of vertical fractures above and below the HD may persist after cooldown, indicating that fracture permeability will be enhanced in these regions. In addition, predicted behavior during cooldown shows increasing hysteresis in displacement with increasing distance from the drift.

Results indicate that fixed displacement boundaries are most appropriate for vertical faces perpendicular to the heated drift. These results provide confidence that the model can be used to predict behavior for an emplacement drift in a nuclear waste repository or other thermally driven fractured rock system.

6. REFERENCES

1. Datta, R.N., S. C. Blair, W. Boyle, R. Finley, M. Peters, Y. Tsang, 1999, "Investigating Coupled Thermal-Mechanical-Hydrological-Chemical Processes in the Drift Scale Test, at Yucca Mountain, Nevada, USA" in Proceedings of 1999 International Society for Rock Mechanics Congress, Paris, France August 1999.

2. Nitao, J.J. 1993. "The NUFT Code for Modeling Nonisothermal, Multiphase, Multicomponent Flow and Transport in Porous Media." *EOS*, 74, (43), 313. Washington, D.C.: American Geophysical Union.

3. Itasca Consulting Group, Inc. 1998. *3DEC, 3 Dimensional Distinct Element Code, User's Guide, (Version 2.00)*. Minneapolis, Minnesota: Itasca Consulting Group.

4. Blair, S. C., S. R. Carlson, and J. L. Wagoner, 2001, "Distinct Element Modeling of the Drift Scale Test", in Rock Mechanics in the National Interest, Proceedings of the 38th U. S. Rock Mechanics Symposium, D. C. Rocks, (pp 527-539), Elsworth, Tinucci and Heasley (eds) July 7-10, 2001 Washington DC/USA Swets & Zeillinger Lisse, ISBN 90 2651 827 7.

5. CRWMS M&O 2001. *Coupled Thermal-Hydrologic-Mechanical Effects on Permeability Analysis and Models Report*. ANL-EBS-HS 000037 Rev 00. Las Vegas, Nevada: CRWMS M&O.

6. Lin, W. et al. 2001 "Large Block Test Final Report", UCRL-ID- 132246 rev2, Dec 2001, Lawrence Livermore National Laboratory, Livermore, CA.

7. Brodsky, N. S., et al., 1997, "thermal expansion, thermal conductivity and Heat Capacity Measurements for Boreholes UE25-NRG-4, UE25-NRG-5, USW-NRG-6 and USW- NRG-7/7A DSNF95-1955. Albuquerque NM: Sandia National Laboratory.

DAB000000-01717-5700-00003 REV 00 ICN 1. Las Vegas, Nevada: CRWMS M&O.